Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 317 °C

Global applicability domain: Outside

Local applicability domain index: 1.20e-01

Confidence level: 6.86e-01

Nearest Neighbors from the Training Set

Image not found
Ametryn
Measured: 345
Predicted: 341

Image not found
Desmetryn
Measured: 345
Predicted: 341

Image not found
2,4,6-Tricyano-1,3,5-triazine
Measured: 262
Predicted: 264

Image not found
Carfentrazone-ethyl
Measured: 353
Predicted: 350

Image not found
2,7,8,9-Tricyclazole
Measured: 275
Predicted: 290